# Nonhomogenous patterns with core defects in elongational flows of liquid crystal polymers

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**Synopsis**

The interaction between flow and orientation of liquid crystalline polymers (LCPs) creates remarkable heterogeneous patterns in which defects, or singular solutions, serve to mediate a confluence of ordered nematic phases. The origin of defects remains a mystery. It is therefore valuable to have models for LCP flows that provide some evidence of defects, and of the corresponding physical competition between flow and LCP properties. In this direction, the flow-orientation moment-averaged Doi model is studied with an imposed elongational flow. Nonhomogeneous, biaxial nematic patterns are discovered in both axial and planar elongation. These exact solutions consist of spatially varying directors in the plane orthogonal to the flow axis, coupled with homogeneous biaxial order parameter equilibria fixed by the LCP concentration ($N$) and elongation rate ($\nu$). For each $(N,\nu)$, the following patterns coexist all with identical order parameter values: the homogeneous patterns of Rey [Macromol. Theory Simul. **4**, 857–872 (1995)]; radially symmetric director patterns; and finally, director patterns periodic in the cylindrical azimuthal angle. The nonhomogeneous structures are distinguished by the presence of core defects along the axis of flow symmetry, characterized by a logarithmic pressure singularity at the core. © *1999 The Society of Rheology.* [S0148-6055(99)01506-0]

## I. INTRODUCTION

The moment-averaged Doi theory with a short-range elastic potential provides a good model for analyzing local homogeneous patterns and phase transitions, in which the averaged molecular orientation is characterized through an orientation tensor (a second order, symmetric, traceless tensor) [Doi (1980), (1981)]. From this theory, See *et al.* (1990), Hu and Ryskin (1991; 1992), Sonnet *et al.* (1995), Bhave *et al.* (1993) studied flow-induced phase transitions for spatially homogeneous uniaxial equilibria in shear and/or elongation. Khokhlov and Semenov (1982) used a similar theory with the Onsager potential. In a seminal paper Rey (1995) discovered spatially homogeneous biaxial patterns in elongational flows and discussed their bifurcation behavior in terms of the two order parameters of the orientation tensor **Q**. This analysis assumes a fixed set of directors, with one director aligned with the flow axis of symmetry.

Here we seek spatially nonhomogeneous patterns in elongational flow. To do so, we recast the Doi model in cylindrical coordinates. This allows us to identify a class of

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solutions with the identical order parameter values as in Rey (1995), with one director again aligned with the flow axis, but where the remaining director angle in the plane orthogonal to the flow axis is allowed to vary as a function of the azimuthal angle. For homogeneous orientation tensors with simple elongational flow, the momentum equation is satisfied automatically. However, *nonhomogeneous structures* feed back to the momentum balance through gradients of the orientation tensor $\mathbf{Q}$. We show conservation of momentum can be maintained by discrete choices for the director angle as a function of the cylindrical polar coordinate. These nonhomogeneous patterns suffer a logarithmic singularity in pressure along the flow axis of symmetry, and therefore constitute exact solutions of the Doi flow-orientation model with a core defect. The potential role of these defect structures in physical experiments is yet to be determined.

## II. THE CONSTRUCTION OF NONHOMOGENEOUS DIRECTOR PATTERNS

We begin with a brief review of the moment-averaged (approximate) Doi theory with short range Maier–Saupe potential formulated by Bhave *et al.* (1993), in which flows are treated as incompressible, $\nabla\cdot\mathbf{v} = 0$. The balance of momentum, constitutive equation for the extra stress, and nematodynamic equation involve the orientation tensor, defined by

$$\mathbf{Q} = \langle \mathbf{m}\otimes\mathbf{m}\rangle - \mathbf{I}/3, \tag{1}$$

where $\mathbf{m}$ is a unit vector in the liquid crystal polymer (LCP) molecular direction, and the average $\langle(\bullet)\rangle$ is with respect to a molecular probability density function consistent with rigid rod molecules. The model equations are given by Bhave *et al.* (1993)

$$\rho\frac{d}{dt}\mathbf{v} = \nabla\cdot(-p\mathbf{I}+\tau), \tag{2a}$$

$$\tau = 2\eta\mathbf{D} + 3ckT[F(\mathbf{Q}) + 2\lambda(\nabla\mathbf{v}:\mathbf{Q})(\mathbf{Q}+\mathbf{I}/3)], \tag{2b}$$

$$\frac{d}{dt}\mathbf{Q} - (\nabla\mathbf{v}\cdot\mathbf{Q} + \mathbf{Q}\cdot\nabla\mathbf{v}^T) = \frac{2}{3}\mathbf{D} - 2(\nabla\mathbf{v}:\mathbf{Q})(\mathbf{Q}+\mathbf{I}/3) - \frac{1}{\lambda}F(\mathbf{Q}), \tag{2c}$$

$$F(\mathbf{Q}) = (1-N/3)\mathbf{Q} - N(\mathbf{Q}\cdot\mathbf{Q}) + N(\mathbf{Q}:\mathbf{Q})(\mathbf{Q}+\mathbf{I}/3), \tag{2d}$$

where $\rho$ is the density of the polymeric liquid, $\mathbf{v}$ is the velocity, $\tau$ is the extra stress tensor, $d/dt$ denotes the material derivative, $\mathbf{D} = \frac{1}{2}[\nabla\mathbf{v} + \nabla\mathbf{v}^T]$ is the rate-of-strain tensor, $p$ is the pressure, $\eta$ is the solvent viscosity, $\lambda$ is the relaxation time associated with rotation of the dumbbell molecules, $c$ is the number of polymer molecules per unit volume, $N$ is the dimensionless polymer concentration which measures the strength of the intermolecular short-range Maier–Saupe potential, $k$ is the Boltzmann constant, and $T$ is absolute temperature. In this study, external forces are ignored.

We note that the general orientation tensor $\mathbf{Q}$, defined by Eq. (1), is a symmetric, traceless, rank two tensor. This means that once coordinates are specified, $\mathbf{Q}$ is represented as a symmetric, traceless, $3\times 3$ matrix with five independent components in general.

We are interested in orientation structures that exist in response to an imposed simple elongational velocity field:

$$\mathbf{v} = \nu\left(-\frac{x}{2},-\frac{y}{2},z\right), \tag{3}$$

with gradient

$$\nabla\mathbf{v} = \nu\,\mathrm{diag}(-\tfrac{1}{2},-\tfrac{1}{2},1), \tag{4}$$

in rectangular coordinates $(x,y,z)$ with respect to the basis $(\mathbf{e}_x,\mathbf{e}_y,\mathbf{e}_z)$. For $\nu > 0$, the flow stretches along the $z$ axis, called axial or unidirectional elongation; for $\nu < 0$, the flow stretches radially in the entire plane orthogonal to the $z$ axis, called planar or bidirectional elongation. With this imposed flow, the Doi model, Eq. (2), admits exact uniaxial and biaxial homogeneous steady patterns with the eigenvectors of $\mathbf{Q}$ aligned with the coordinate basis [Rey (1995)]. We remark further that these steady patterns are invariant under arbitrary rotation of the directors in the plane transverse to the flow axis of symmetry $(\mathbf{e}_z)$. That is, $\mathbf{V}_\zeta\mathbf{Q}_0\mathbf{V}_\zeta^T$ is a steady pattern provided $\mathbf{Q}_0$ is, where

$$\mathbf{V}_\zeta = \begin{pmatrix} \cos\zeta & \sin\zeta & 0 \\ -\sin\zeta & \cos\zeta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \zeta \text{ arbitrary.} \tag{5}$$

All of these homogeneous steady states $\mathbf{Q}_0$ have one director parallel to the flow axis $\mathbf{e}_z$. This construction prompts us to seek nonhomogeneous solutions of the Doi model exhibiting radial symmetry in the plane transverse to the flow direction.

To do so, we first cast the Doi model, Eq. (2), in cylindrical coordinates $(r,\theta,z)$, with the $z$ axis coincident with the flow direction. The flow field, Eq. (3), takes the form

$$\mathbf{v} = \nu\left(-\frac{r}{2},0,z\right), \tag{6}$$

with gradient

$$\nabla\mathbf{v} = \nu\,\mathrm{diag}(-\tfrac{1}{2},-\tfrac{1}{2},1), \tag{7}$$

in cylindrical coordinates $(r,\theta,z)$ with respect to the basis $(\mathbf{e}_r,\mathbf{e}_\theta,\mathbf{e}_z)$. Note the velocity gradient $\nabla\mathbf{v}$ is *identical* in both coordinate systems. A critical issue in this study is the consistency of the momentum balance, Eq. (2a), which for homogeneous $\mathbf{Q}$ is trivially satisfied because the orientation contribution to stress is constant in space. However, for nonhomogeneous orientation structures, the momentum equation (2a) with $\mathbf{v}$ given by Eqs. (3) or (6) translates into a tensorial partial differential equation coupling pressure $p$ and orientation tensor $\mathbf{Q}$.

We now construct a special class of solutions of the coupled flow-nematic equations with orientation tensor $\mathbf{Q}$ of the form

$$\mathbf{Q} = \mathbf{V}_\zeta\left[s\left(\mathbf{e}_z\otimes\mathbf{e}_z-\frac{\mathbf{I}}{3}\right)+\beta\left(\mathbf{e}_r\otimes\mathbf{e}_r-\frac{\mathbf{I}}{3}\right)\right]\mathbf{V}_\zeta^T = s\left(\mathbf{n}_3\otimes\mathbf{n}_3-\frac{\mathbf{I}}{3}\right)+\beta\left(\mathbf{n}_2\otimes\mathbf{n}_2-\frac{\mathbf{I}}{3}\right), \tag{8}$$

with the following properties:

(i) one director ($\mathbf{n}_3 = \mathbf{V}_\zeta \mathbf{e}_z = \mathbf{e}_z$) is fixed parallel to the flow axis of symmetry;

(ii) the remaining two orthogonal directors (eigenvectors) of $\mathbf{Q}$ lie in the plane perpendicular to $\mathbf{e}_z$, and vary in space and time through the single director angle $\zeta = \zeta(\theta,t)$; this is made explicit by the relations

$$\mathbf{n}_2 = \mathbf{V}_\zeta \mathbf{e}_r, \quad \mathbf{n}_1 = \mathbf{V}_\zeta \mathbf{e}_\theta; \tag{9}$$

(iii) the two independent order parameters $s = s(t)$, $\beta = \beta(t)$, do not vary in space.

Note steady states constructed below from this form of $\mathbf{Q}$ will have uniform degrees of orientation at each location, but with spatial nonhomogeneity through variation of the directors (principal axis of orientation).

Since $\nabla \mathbf{v}$ is a diagonal constant matrix, the nematodynamic equation (2c) collapses to a tensorial ordinary differential equation in time, where the spatial coordinate $\theta$ enters parametrically, *if* the convective transport term vanishes,

$$(\mathbf{v}\cdot\nabla)\mathbf{Q} = \nu\left(-\frac{r}{2}\frac{\partial}{\partial r} + z\frac{\partial}{\partial z}\right)\mathbf{Q} = \mathbf{0}. \tag{10}$$

The special form of $\mathbf{Q}$, Eqs. (8)–(9), is posited precisely to satisfy this condition. Thus, the nematodynamic equation (2c) becomes an ordinary differential equation for the class of $\mathbf{Q}$ defined by Eqs. (8)–(9)

$$\begin{cases} \dot{\mathbf{Q}} = -\dfrac{1}{\lambda}F(\mathbf{Q}) + G(\mathbf{Q};\nabla\mathbf{v}), \\[2ex] G(\mathbf{Q};\mathbf{D}) = \mathbf{D}\mathbf{Q} + \mathbf{Q}\mathbf{D} + \dfrac{2}{3}\mathbf{D} - 2\mathbf{D}:\mathbf{Q}\left(\mathbf{Q} + \dfrac{\mathbf{I}}{3}\right), \\[2ex] \mathbf{D} = \nu\,\mathrm{diag}(-1/2,-1/2,1). \end{cases} \tag{11}$$

At this point, we have the time dependence of the order parameters $s$, $\beta$ and director angle $\zeta$ governed by the nematic dynamics, Eq. (11), coupled with the momentum equation (2a) governing the pressure $p$. We now analyze the constraints imposed by (2a), which in component form yields

$$\frac{1}{4}\rho\,\nu^2 r = -p_{,r} + \tau_{rr,r} + \frac{1}{r}(\tau_{rr} - \tau_{\theta\theta} + \tau_{r\theta,\theta}) + \tau_{rz,z}, \tag{12a}$$

$$0 = -\frac{1}{r}p_{,\theta} + \frac{1}{r^2}(r^2\,\tau_{r\theta})_{,r} + \frac{1}{r}\tau_{\theta\theta,\theta} + \tau_{\theta z,z}, \tag{12b}$$

$$\rho\nu^2 z = -p_{,z} + \frac{1}{r}(r\tau_{rz})_{,r} + \tau_{zz,z} + \frac{1}{r}\tau_{\theta z,\theta}, \tag{12c}$$

where the notation $()_{,a}$ denotes partial derivative with respect to $a$. The extra stress components follow from the Doi constitutive relation (2b) and the special form of $\mathbf{Q}$, Eqs. (8)–(9):

$$\tau_{rr} = -\eta\nu + 3ckT\left[-\frac{U(s)}{3} + \frac{U(\beta)}{6} + \frac{Ns\beta}{9}(3s-3\beta-1)\right] + 3ckT\lambda\nu\left(\frac{2s}{3} - \frac{2s^2}{3} + \frac{2s\beta}{3} - \frac{\beta^2}{6} - \frac{\beta}{3}\right) + \left\{3ckT\left[U(\beta) + \frac{2Ns\beta}{3}(1+s-\beta)\right] + \alpha\lambda\nu(2s\beta-\beta^2)\right\}\frac{\cos 2\zeta}{2}, \tag{13a}$$

$$\tau_{\theta\theta} = -\eta\nu + 3ckT\left[-\frac{U(s)}{3} + \frac{U(\beta)}{6} + \frac{Ns\beta}{9}(3s-3\beta-1)\right] + 3ckT\lambda\nu\left(\frac{2s}{3} - \frac{2s^2}{3} + \frac{2s\beta}{3} - \frac{\beta^2}{6} - \frac{\beta}{3}\right) - \left\{3ckT\left[U(\beta) + \frac{2Ns\beta}{3}(1+s-\beta)\right] + 3ckT\lambda\nu(2s\beta-\beta^2)\right\}\frac{\cos 2\zeta}{2}, \tag{13b}$$

$$\tau_{zz} = -(\tau_{rr} + \tau_{\theta\theta}) + \lambda\nu 3ckT(2s-\beta), \tag{13c}$$

$$\tau_{r\theta} = 3ckT\left\{U(\beta) + \frac{2Ns\beta}{3}(1+s-\beta) + \lambda\nu(2s\beta-\beta^2)\right\}\frac{\sin 2\zeta}{2}, \tag{13d}$$

$$\tau_{rz} = 0, \quad \tau_{\theta z} = 0,$$

where

$$U(s) = s\left[1 - \frac{N}{3}(1-s)(2s+1)\right] \tag{14}$$

gives the uniaxial bulk free energy $\int U(s)\,ds$.

Note that

$$\tau_{rr} - \tau_{\theta\theta} + \tau_{r\theta,\theta} = 3ckT\left[U(\beta) + \frac{2Ns\beta}{3}(1+s-\beta) + \lambda\,\nu(2s\beta-\beta^2)\right]\cos(2\zeta)(1+\zeta_{,\theta}),$$
$$\tau_{rr,r} = 0. \tag{15}$$

The radial momentum balance, Eq. (12a) yields

$$p_{,r} = -\frac{\rho}{4}\nu^2 r + \frac{3ckT}{r} f(s,\beta)\cos(2\zeta)\,(1+\zeta_{,\theta}), \tag{16}$$

where

$$f(s,\beta) = U(\beta) + \frac{2N}{3}s\beta(1+s-\beta) + \lambda\nu(2s\beta-\beta^2). \tag{17}$$

Thus the pressure has a potential $\ln(r)$ singularity along the axis of flow symmetry, $r = 0$.

First we pursue elimination of the $\ln(r)$ singularity in pressure, which requires one of the following conditions to be satisfied:

$$f(s,\beta) = 0, \tag{18}$$

$$1 + \zeta_{,\theta} = 0, \tag{19}$$

$$\cos 2\zeta = 0. \tag{20}$$

The first condition, Eq. (18), forces $\beta = 0$, a uniaxial limit in which $\mathbf{Q}$ collapses to a spatially homogeneous form $s(t)[\mathbf{e}_z \otimes \mathbf{e}_z - (\mathbf{I}/3)]$. The second condition, Eq. (19) implies $\zeta = -\theta + \zeta_0(t)$, *which recovers the spatially homogeneous* form of $\mathbf{Q}$ employed by Rey (1995). Further analysis of the momentum equation yields a finite pressure field everywhere:

$$p = -\frac{1}{8}\rho\nu^2 r^2 - \frac{\rho}{2}\nu^2 z^2 + \bar{p}(t). \tag{21}$$

The final choice, Eq. (20), yields *discrete* radially symmetric patterns, with $\zeta = \pi/4 \bmod \pi/2$, where the pressure is given by

$$p = -\frac{1}{8}\rho\nu^2 r^2 - \frac{\rho}{2}\nu^2 z^2 + \bar{p}(t) + 2\tau_{r\theta}\theta. \tag{22}$$

However, this pressure is multiple valued and therefore physically ill-defined unless $\tau_{r\theta}$ vanishes. From Eq. (13d) we impose $\tau_{r\theta} = 0$, which gives $\zeta = 0 \bmod \pi/2$, in contradiction to the previous condition $\zeta = \pi/4 \bmod \pi/2$.

In summary, elimination of the $\ln r$ pressure singularity leads only to previously identified spatially homogeneous patterns [Rey (1995)].

Next we explore exact solutions that allow the $\ln(r)$ pressure singularity. We begin by integrating the angular momentum equation (12b), which has ill-defined terms *unless* the following conditions are met:

$$\int_0^{2\pi} \sin 2\zeta(\theta) d\theta = 0, \quad \cos 2\zeta(\theta + 2\pi) = \cos 2\zeta(\theta). \tag{23}$$

We then integrate the radial momentum equation and find that an ill-defined term appears *unless*

$$\cos 2\zeta(\theta+2\pi)[1+\zeta_{,\theta}(\theta+2\pi)] = \cos 2\zeta(\theta)[1+\zeta_{,\theta}(\theta)]. \tag{24}$$

Finally integrating the axial momentum equation yields

$$p = -\frac{1}{8}\rho\nu^2 r^2 - \frac{\rho}{2}\nu^2 z^2 + \ln(r) 3ckTf(s,\beta)\cos 2\zeta(\theta)(1+\zeta_{,\theta}) + 3ckTf(s,\beta)\int_0^{\theta} \sin 2\zeta(\theta) d\theta$$
$$+ \tau_{\theta\theta} - \tau_{\theta\theta}(\theta = 0) + \bar{p}(t). \tag{25}$$

We do not yet have a complete classification of all functions $\zeta(\theta)$ which satisfy the relations, Eqs. (23)–(24). Nonetheless, our construction yields successful exact patterns if we can produce any such functions. Indeed, the following discrete family of functions $\zeta(\theta)$ satisfies Eqs. (23) and (24):

$$\zeta(\theta) = n\theta + \zeta_0, \quad n = \pm 1, \pm 2, \ldots, \tag{26}$$

$$\zeta_0 \text{ constant}$$

or

$$\zeta = 0 \bmod \frac{\pi}{2}. \tag{27}$$

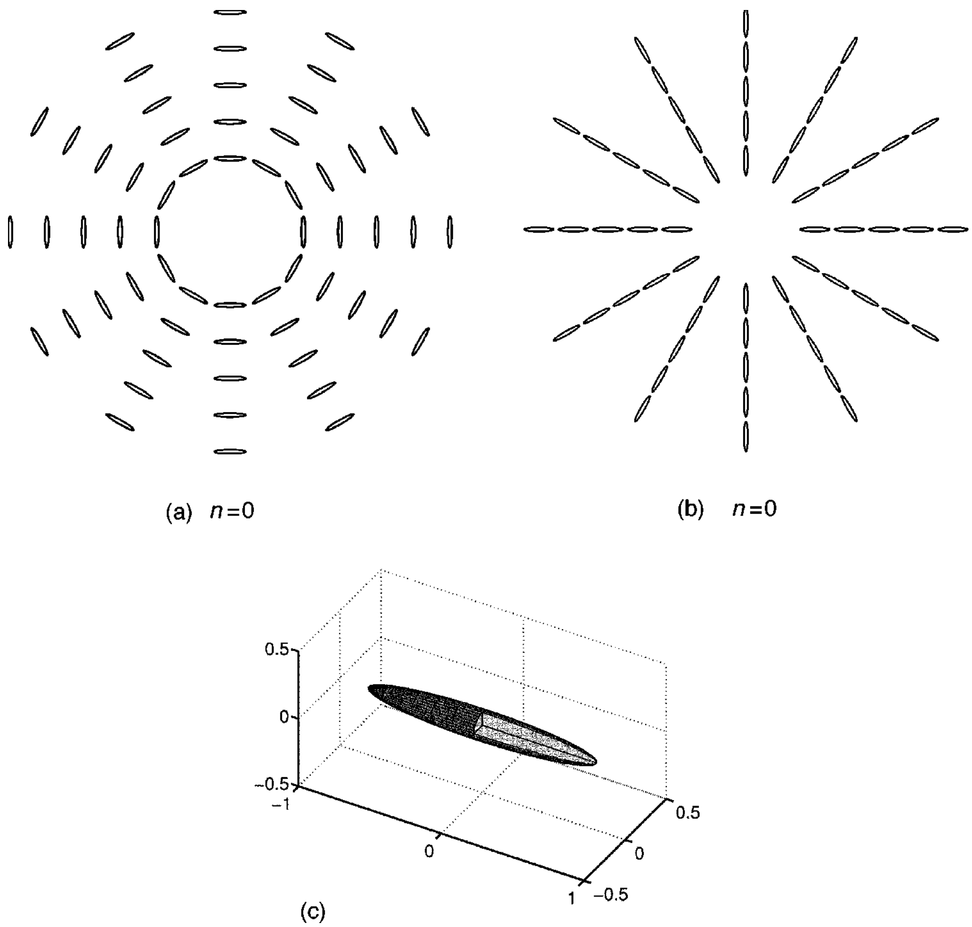


**FIG. 1.** Biaxial steady orientation patterns in the plane transverse to the axis of flow symmetry. The dimensionless concentration $N = 4$, whereas the planar elongational rate relative to polymer relaxation time is $\lambda\nu = -0.1$. All patterns correspond to core defects with a $\ln(r)$ pressure singularity at $r = 0$. In (a) the degree of orientation variables with respect to the two in-plane directors $\mathbf{n}_2 = \mathbf{e}_\theta$, $\mathbf{n}_1 = \mathbf{e}_r$, are $d_2 = 8.802$, $d_1 = 0.104$, respectively, where $\mathbf{n}_2$ is the major director. In (b), $d_1 = 0.802$, $d_2 = 0.104$ and the major director is $\mathbf{n}_1$. These two orientation patterns are related by a 90° in-plane rotation. (c) Is a blow up of the orientation tensor represented by an ellipsoid.

The patterns for given $n$ (except $n = -1$) in Eq. (26) have period $\pi/(n+1)$ radians in the $r-\theta$ plane.

With the momentum equation balanced, with pressure $p$ given by Eq. (25), $\zeta$ given by Eqs. (26) or (27), $\mathbf{v}$ prescribed by Eq. (6), the remaining order parameter unknowns $s(t)$, $\beta(t)$ are given by the ode Eq. (11) which collapses to that studied by Rey (1995). Thus all biaxial order parameter steady states, performed in the completely different context of homogeneous elongation-induced patterns, further define nonhomogeneous biaxial patterns by the above construction. The existence of biaxial patterns varies with the LCP concentration parameter $N$ and the product $\lambda\nu$ of polymer relaxation time $\lambda$ and elongation rate $\nu$, the so-called Peclet number (Pe).

In summary, we have constructed a discrete family of exact steady orientation patterns with a $\ln r$ pressure singularity (except for $n = -1$; see below) that we call a core defect. The $\mathbf{Q}$ tensor is constructed from the biaxial equilibria $(s,\beta)$ vs $N$,Pe from Rey (1995).

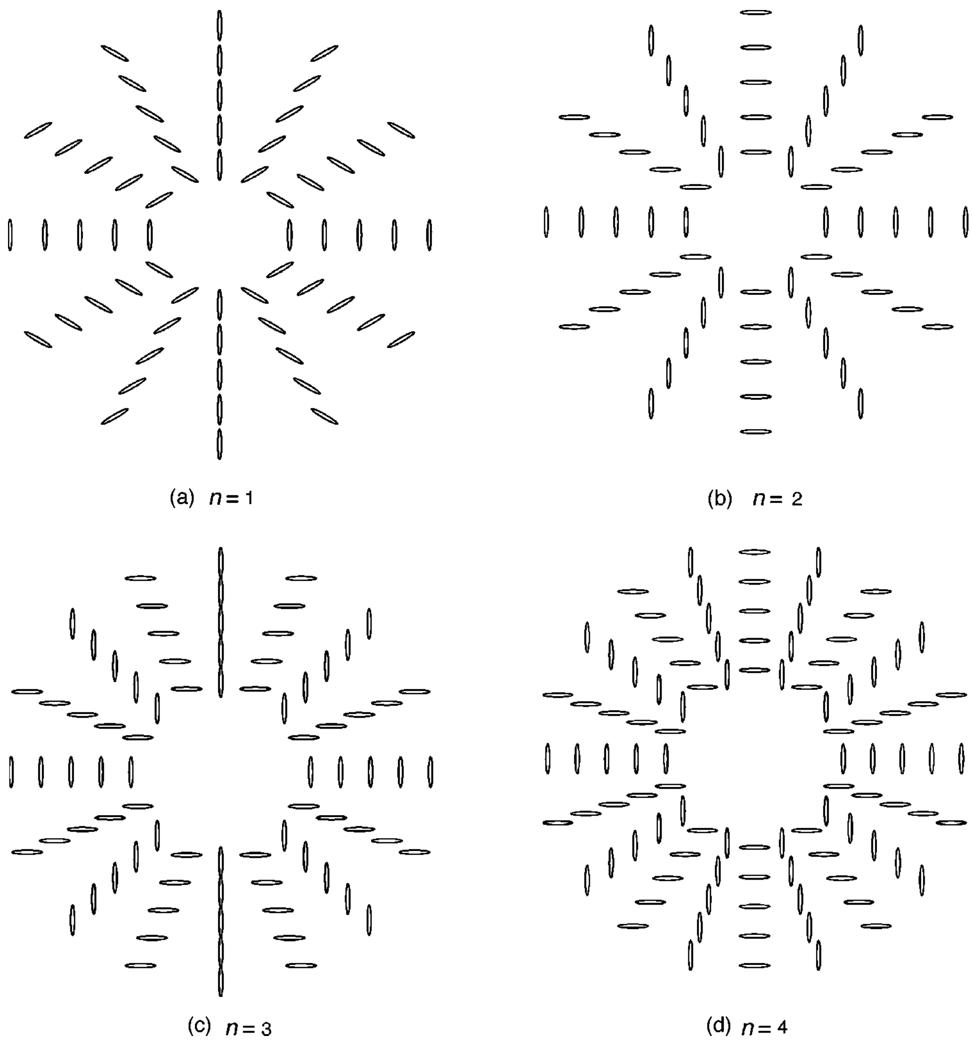


**FIG. 2.** Nonhomogeneous biaxial patterns for Pe $= -0.1$, $N = 4$.

The steady state values $(s,\beta)$ for given $(N,\mathrm{Pe})$ determine the direction cosines $d_i = \langle \cos^2\phi_i \rangle$ [Forest *et al.* (1997)],

$$d_1 = (1-s-\beta)/3, \quad d_2 = (1-s+2\beta)/3, \quad d_3 = 1-d_1-d_2, \tag{28}$$

where $\langle\,\rangle$ is with respect to the probability distribution function of the Doi theory, $\phi_i$ is the angle between the rod-like molecule axis $\mathbf{m}$ and director $\mathbf{n}_i$. We use this order parameter and director information to construct the local orientation at each spatial location in the form of an ellipsoid [see Fig. 1(c)] with major axes $\mathbf{n}_i$ and semiaxis lengths $d_i$. Since all patterns constructed here have $\mathbf{n}_3 = \mathbf{e}_z$, all information except the semiaxis length $d_3$ is conveyed by the two dimensional projection of these ellipsoids onto the plane transverse to the flow axis of symmetry.

We now describe specific members of this family.

For $n = -1$, the $\ln r$ singularity vanishes and the spatially homogeneous form of $\mathbf{Q}$ [Rey (1995)] is recovered. [While not necessarily obvious, if the director angle $\zeta$

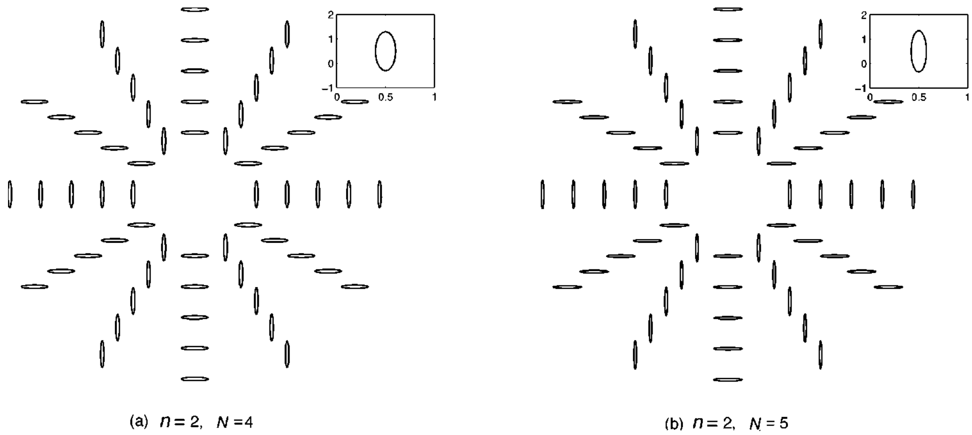


**FIG. 3.** Nonhomogeneous patterns for different concentrations ($N$) where Pe $= -0.1$. The degrees of orientation fix the semiaxes of length $d_1 = 0.104$, $d_2 = 0.802$, $d_3 = 0.094$ in (a), and $d_1 = 0.0786$, $d_2 = 0.8485$, $d_3 = 0.0729$ in (b). The spatial inhomogeneity is due to periodicity with respect to the angle coordinate ($\theta$) in the plane transverse to the flow axis of symmetry.

$= -\theta+\zeta_0$, the directors $\mathbf{n}_1$, $\mathbf{n}_2$ in Eq. (9) become a constant rotation by $\zeta_0$ of $\mathbf{e}_x$, $\mathbf{e}_y$. Thus the tensor $\mathbf{Q}$ becomes spatially homogeneous.]

For all other $n \neq -1$, the $\ln r$ pressure singularity persists.

The special case $\zeta = 0 \bmod \pi/2$ yields two discrete *radially symmetric* orientation patterns with a core defect. The radial symmetry occurs because the directors are locked with the coordinate vectors. Figure 1 depicts two biaxial patterns for $\zeta = 0$ and $\pi/2$, respectively, for a given Péclet number (Pe $= \nu\lambda = -0.1$) and concentration parameter $N = 4$.

Figure 2 gives nonhomogeneous biaxial patterns for $n = 1,2,3,4$, respectively, with $N = 4$, Pe $= -0.1$ as in Fig. 1.

Figure 3 illustrates the change of the local degrees of orientation, $d_i$, by variation of the concentration parameter $N$, for fixed Pe. By fixing $n = 2$, the spatial variation of the local orientation ellipsoid is identical for each figure, so only the local ellipsoid shape varies. The corresponding *homogeneous* patterns for these same $(N,\mathrm{Pe})$, with these identical steady order parameter values (therefore the same semiaxes $d_i$), and with arbitrary direction $\mathbf{n}_1$, $\mathbf{n}_2$ in the $r-\theta$ plane, are *neutrally stable*.

## III. CONCLUSION

In the study of spatially homogeneous orientation patterns in response to pure elongational flow, the momentum equation of the Doi theory is trivially satisfied. If one considers nonhomogeneous patterns with prescribed pure elongation, then the momentum balance yields constraints on the remaining unknowns: the pressure and the orientation tensor. Here we have constructed special orientation structures which in the simplest case recover the spatially homogeneous, elongation-induced patterns of Rey (1995), for which the pressure is finite and well behaved. Further exact solutions of the full Doi momentum-nematic equations are constructed which retain the equilibrium order parameter values of Rey's homogeneous patterns, but embellish Rey's constant directors by admitting an azimuthal dependence of the directors in the plane orthogonal to the flow axis of symmetry. The simplest of the nonhomogeneous structures yields two discrete, radially symmetric, biaxial director patterns that coexist with homogeneous biaxial patterns at fixed values of LCP concentration and elongation rate. These exact constructions are distinguished by the occurrence of a $\ln r$ singularity in the pressure, where $r$ is the radial coordinate in the plane orthogonal to the flow axis. We call these patterns core defects because of the combined director confluence and pressure singularity along the core, or axis of flow symmetry. We recall from Rey (1995) that for bidirectional elongation, above a moderate LCP concentration the only stable patterns are biaxial. Thus these core defects inherit the stability to pure order parameter perturbations, that is, to perturbations in the degrees of orientation. The more difficult and physically relevant question of whether there exist patterns which approximate these nonhomogeneous structures, but with some regularization of the core singularity, remains open. Nonetheless, it is remarkable that the Doi theory captures these exact solutions exhibiting core defects.

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## References

Bhave, A. V., R. K. Menon, R. C. Armstrong, and R. A. Brown, ''A constitutive equation for liquid crystalline polymer solutions,'' J. Rheol. **37**, 413–441 (1993).

Doi, M., ''Rheological properties of rodlike polymers in isotropic and liquid crystalline phases,'' Ferroelectrics **30**, 247–254 (1980).

Doi, M., ''Molecular dynamics and rheological properties of concentrated solutions of rodlike polymers in isotropic and liquid crystalline phases,'' J. Polym. Sci., Polym. Phys. Ed. **19**, 229–243 (1981).

Forest, M. G., Q. Wang, and S. Bechtel, ''One-dimensional isothermal spinning models for liquid crystalline polymer fibers,'' J. Rheol. **41**, 821–850 (1997).

Hu, T. and G. Ryskin, ''Numerical simulation of rodlike polymers in a uniaxial extensional flow: The distribution-function version versus the order-parameter version of Doi's theory,'' J. Chem. Phys. **95**, 6042–6049 (1991).

Hu, T. and G. Ryskin, ''Numerical simulation of rodlike polymers in extensional and sink/source flows using the order-parameter version of Doi's theory,'' J. Chem. Phys. **96**, 4705–4717 (1992).

Khokhlov, A. and A. Semenov, ''Influence of external field on the liquid-crystalline ordering in solutions of stiff-chain macromolecules,'' Macromolecules **15**, 1272–1277 (1982).

Rey, A., ''Bifurcational analysis of the isotropic-nematic phase transition of rigid rod polymers subjected to biaxial stretching flow,'' Macromol. Theory Simul. **4**, 857–872 (1995).

See, H., M. Doi, and R. G. Larson, ''The effect of steady flow fields on the isotropic-nematic phase transition of rigid rod-like polymers,'' J. Chem. Phys. **92**, 792–800 (1990).

Sonnet, A, A. Kilian, and S. Hess, ''Alignment tensor versus director: Description of defects in nematic liquid crystals,'' Phys. Rev. E **52**, 718–722 (1995).